The thermodynamic cost of reliability and low temperatures: Tightening Landauer's principle and the Second Law

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Landauer's principle states that the erasure of one bit of information requires the free energy $kT \ln 2$. We argue that the reliability of the bit erasure process is bounded by the accuracy inherent in the statistical state of the energy source ('the resources') driving the process. We develop a general framework describing the 'thermodynamic worth' of the resources with respect to *reliable bit erasure* or *good cooling*. This worth turns out to be given by the distinguishability of the resource's state from its equilibrium state in the sense of a statistical inference problem. Accordingly, Kullback-Leibler relative information is a decisive quantity for the 'worth' of the resource's state. Due to the asymmetry of relative information, the reliability of the erasure process is bounded rather by the relative information of the *equilibrium state with respect to the actual state* than by the relative information of the *actual state with respect to the equilibrium state* (which is the free energy up to constants).

I. INTRODUCTION

One of the characteristic features of technological progress is the increase of human ability to control and design the microscopic world. Especially the recent successes in manipulating simple quantum systems (for example in the context of Quantum Computing research) are one aspect of this general development. Since every process controlling microscopic particles is disturbed by heat, this progress is strongly connected with the invention of efficient *cooling mechanisms* (see [1], [2], [3]). This statement is in some sense[1] a *tautological* one: Preparing a physical system in a *pure* quantum state means preparing a state *without entropy*, i.e., a system *without heat*. In present day cooling techniques, the size of the required apparatus is quite impressive compared to the tininess of the cooled systems. In contrast, miniaturization in computer technology will require smaller, efficient and power saving mechanisms for draining off entropy on the nanoscopic or microscopic level. This raises the question for fundamental lower bounds on the resources needed for cooling simple quantum systems. At first sight the answer seems to be given by well-known thermodynamic theory, in particular the Second Law: Extracting the entropy S from a system requires the energy $S\,kT$ where k is Boltzmann's constant and T the temperature of the surrounding heat bath absorbing the entropy. Another formulation of this law is Landauer's principle saying that the erasure or initialization of one bit being in an unknown state requires at least the energy $\ln 2\, kT$ (see [4], [5], [6]). But this cannot be the complete answer: To understand the fundamental limitations on scaling down the cooling apparatus and reducing the resources, we model the cooling process as an energy conserving unitary dynamics on the composition of the considered quantum system with another one ('the resources'). Within this microscopic model we do not expect that necessary *and sufficient* conditions for the resource's quantum state to enable effective cooling procedures are given by well-known laws of thermodynamics.

Of course, a lot of steps have already been made towards a refinement of thermodynamics on the level of low-dimensional quantum systems (see e.g. [7], [8]). Actually, one should reckon all the results concerning entanglement purification [9], quantum error correction [10] [11], quantum data compression [12], and logical cooling [13] as such since they are dealing essentially with the *transport* and *concentration* of information by operations on compositions of simple quantum systems. Nevertheless, our approach is rather different from those ones: Our microphysical models of cooling include the energy source – a quantum system as well – driving the process, i.e., we restrict the class of unitary transformations to those conserving the total Hamiltonian of the system. This setup emphasizes the fact, that we want to develop a theory of *thermodynamics* in contrast to a pure theory of *information*: The latter one deals with *information* only, while the first one focuses on the *relation between energy and information*.

Some consequences of the restriction to energy conserving transformations can be illustrated easily: Consider a bipartite quantum system consisting of a harmonic oscillator with frequency ν and a two-level system with energy levels 0 and $h\nu$. Assume both systems to be in their equilibrium states for the same (finite) temperature. Then one can easily construct unitary transformations on the composite Hilbert space extracting entropy from the

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[1] We use the cautious formulation 'in some sense' because of the following objection: If the system has a large energy gap between its ground state and the first excited state, it is in an almost pure state even for not too low temperatures.

two-level system and pumping into the oscillator. One can even show, that there are no bounds on the efficiency of such a cooling process, i.e., the state of the two-level system can be prepared arbitrarily close to a pure one. In contrast, there is no *energy conserving* unitary transformation changing the state of the system at all. Such a process would even violate the Second Law, since this would be a dynamics producing free energy without the use of an additional energy source. Accordingly, if the state of the harmonic oscillator differs *slightly* from its equilibrium state we will expect that an energy preserving process can only have a *slight* cooling effect. Lead by this intuition, we investigate in which way the size of the deviation of the quantum system's state from its equilibrium state determines its 'thermodynamic worth' for enabling good cooling processes, or more generally, for *precise* preparation of quantum states. Reformulated in the spirit of the 'thermodynamics of computation', we investigate the minimal resource requirements for a *reliable* bit erasure process.

The paper is organized as follows: In section II we give a short introduction into thermal equilibrium states of quantum systems. In section III we present the formal setup of the microscopic cooling process and give necessary and sufficient conditions for the resource's state to allow for cooling a two-level system. In section IV we introduce a more flexible model in which cooling is described by a unitary dynamics on a tripartite system: The resources, the environment being in thermal equilibrium, and the two-level system to be cooled down. We prove that cooling is possible if and only if the time average of the resource's state does not agree with its equilibrium state. If the temperature of the two-level system is already below the environment's temperature, the deviation of the resource's state from equilibrium determines whether it is possible to cool the qubit even more. The second part of this section answers the totally different question of the lowest qubit-temperature which can be obtained by using the given resources if the qubit has initially the same temperature as the environment. We show that the determination of the lowest obtainable temperature can be reduced to a quantum inference problem, namely the determination of error probabilities of a decision rule for distinguishing the resource's state from its equilibrium state. Sections V-VII shows consequences of our theory and analyze in which sense they go beyond well-known laws of thermodynamics.

II. THERMODYNAMIC BACKGROUND

Let $\mathcal{H}$ be the finite or infinite dimensional Hilbert space of a quantum system and H a selfadjoint operator acting on $\mathcal{H}$ representing its Hamiltonian. Then, for any temperature T the density matrix

$$\rho_T := e^{-H/(kT)}/tr(e^{-H/(kT)}),$$

where k is Boltzmann's constant, is called the *thermal equilibrium state* with temperature T provided that $tr(e^{-H/(kT)})$ exists. Note that we do not define temperature as a property of every state, but merely for those of the form described above.

As usual, we will use the inverse temperature defined by $\beta := 1/(kT)$ and consider the class of states

$$\rho_\beta := e^{-\beta H}/tr(e^{-\beta H})$$

for any β with $-\infty \leq \beta \leq \infty$.

In the special case of a non-degenerate two-level system this implies that an inverse temperature can be assigned to any density matrix commuting with the Hamiltonian. For two diagonal-states the state with lower β is the hotter state. The fact, that *heating* up to a value $\beta < 0$ *decreases* the entropy is the well-known phenomenon of temperature inversion [14]. In order to avoid confusion we emphasize that *heating* means here *increasing* the occupation probability for the upper state. This is connected with an *increase* of entropy for $\beta > 0$ and a *decrease* of entropy for $\beta < 0$. This unusual connection between entropy and heat due to temperature inversion might be confusing. However, we will mostly focus on cooling, since the corresponding statements for heating in our sense can be obtained analogously. In contrast, if one considers the maximally mixed state ($T = \infty$) as the hottest one, there is no such analogy and the preparation of the hottest states does not cause any difficulties comparable to the preparation of the coldest one.

Since we want to interpret our results in the context of 'thermodynamics of computation' we keep in mind that a two-level system can be considered as an one-bit-memory and any process producing an (almost) pure state from a mixed one will be considered as an *erasure* process of one unknown bit of information.

In the following sections the dependence of the equilibrium states from the temperature will mostly not be mentioned explicitly, since troughout the paper we fix one common reference temperature $T \neq 0, T \neq \infty$ (and the corresponding inverse temperature β) representing the temperature of the particle's environment.

III. THE MODEL

To investigate the ability of cooling or heating a multilevel quantum system within a precise mathematical framework, we introduce some terminology: Here, a *quantum system* is uniquely characterized by its Hamiltonian H, since it determines in a unique way the corresponding Hilbert space and its dynamics. Up to an irrelevant translation of the energy scale, for any fixed inverse temperature β there is an one-to-one correspondence between the system's Hamiltonian and its equilibrium state. Note that any unitary operator u commutes with H if and only if it commutes with its equilibrium state provided that $\beta \neq 0$ and $\beta \neq \infty$, i.e, a dynamics is

energy conserving if and only if it preserves the equilibrium state.

Every quantum system can be in different statistical states, described by a density matrix acting on the same Hilbert space as the Hamiltonian. We call a system being in a particular statistical state an *object*. More formally we define:

Definition 1

1. *A (quantum)* **system** *is described by a density matrix γ (its 'equilibrium state') acting on a finite dimensional Hilbert space $\mathcal{H}$.*

2. *An* **object** *is a pair (ρ, γ) where ρ is a density matrix describing the actual mixed state of the system. Hence, a system in equilibrium is described by an object of the form*

$$(\gamma, \gamma).$$

Usually we will assume both matrices to have full rank.

3. *For two systems γ and $\tilde{\gamma}$ we define the* **composed system** *as the system determined by the equilibrium state*

$$\gamma \otimes \tilde{\gamma}.$$

4. *For two objects $O := (\rho, \gamma)$ and $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ the* **composed object** *is defined to be*

$$O \times \tilde{O} := (\rho \otimes \tilde{\rho}, \gamma \otimes \tilde{\gamma})$$

5. *If u is a unitary operator acting on $\mathcal{H}$ with $u\gamma u^* = \gamma$, i.e, u is an 'energy conserving reversible dynamics', we define the* **allowed transformation** *T_u on the object $O := (\rho, \gamma)$ by:*

$$T_u((\rho, \gamma)) := (u\rho u^*, \gamma).$$

In abuse of language, we will call u an allowed transformation as well.

6. *If a system $\gamma \otimes \tilde{\gamma}$ is in the state ρ (where ρ is not a tensor product state necessarily), we define the* **restriction** *of the object $O := (\rho, \gamma \otimes \tilde{\gamma})$ to its left, respectively right, component as*

$$O_l := (tr_r(\rho), \tilde{\gamma})$$

and

$$O_r := (tr_l(\rho), \gamma),$$

where tr_l and tr_r denote the partial trace over the left, repectively right, component in the tensor product.

Within this framework, the problem of cooling a two-level system ('qubit') by given resources can be formalized as follows:

Given the arbitrary object O ('the resources') and the qubit $Q := (\sigma, \sigma)$, with

$$\sigma := \frac{1}{1 + e^{-\beta E}} \, diag(1, e^{-\beta E}),$$

where E is the energy gap of the two-level system. Find an allowed transformation T_u on

$$O \times Q$$

which serves as a cooling process for Q, i.e.,

$$(T(O \times Q))_r$$

is a qubit with a lower or higher temperature compared to the initial state σ.

Firstly we will look for those allowed transformations which minimize or maximize the occupation probability for the upper level. Let σ_z be the Pauli matrix

$$\sigma_z := diag(1, -1)$$

and assume the Hamiltonian of the qubit to be

$$\tilde{H} := diag(0, E).$$

Then the occupation probability for the upper level is maximized (respectively minimized) for those transformations u which minimize (respectively maximize) the term

$$tr(u(\rho \otimes \sigma)u^*(1 \otimes \sigma_z)).$$

We find necessary and sufficient conditions for the transformations u to be optimal:

Lemma 1 *Let α be the density matrix of a bipartite system composed of a qubit with equilibrium state σ as above and another arbitrary system with equilibrium state γ, i.e., we have the object*

$$(\alpha, \gamma \otimes \sigma).$$

Let P_i be the spectral projections of $\gamma \otimes \sigma$. Assume that the following two conditions hold:

1. *All the operators $P_j \alpha P_j$ commute with $1 \otimes \sigma_z$,*

   so that we can divide the eigenvalues of the restriction of $P_j \alpha P_j$ to the range of P_j into subsets Γ_+^j and Γ_-^j corresponding to the eigenvectors of $1 \otimes \sigma_z$ with eigenvalues $+1$ and -1, respectively.

2. *The smallest eigenvalue in Γ_+^j is greater than the greatest eigenvalue in Γ_-^j.*

Then there is no allowed transformation u on $O \times Q$ decreasing the occupation probability of the upper state, i.e., we have:

$$tr(u\alpha u^*(1 \otimes \sigma_z)) \geq tr(\alpha(1 \otimes \sigma_z)),$$

for every unitary operator u with $[u, \gamma \otimes \sigma] = 0$.

The Lemma will be proved in the appendix.

For any allowed transformation u we can decide whether there can exist a better one for cooling by setting $\alpha := u(\rho \otimes \sigma)u^*$. Then Lemma 1 gives a criterion whether there can exist a better transformation u'. Furthermore it shows, that the optimal transformation for reducing the probability of the upper state or the lower state can always be chosen in such a way that the reduced density matrix of the qubit is still diagonal after one has performed the unitary transformation u. Therefore we can obtain an equilibrium state with a temperature different from the reference temperature.

We shall use the following notion:

Definition 2 *Let $Q := (\sigma, \sigma)$ be a qubit in its equilibrium state. We say 'the object $O := (\rho, \gamma)$' can be used for cooling Q if there is an allowed transformation T_u on $O \times Q$ such that*

$$tr(u(\rho \otimes \sigma)u^*(1 \otimes \sigma_z)) > tr(\rho\sigma_z).$$

We say that it can be used for heating if we have '$<$' instead of '$>$'.

In order to give necessary and sufficient conditions for the possibility of cooling or heating the following suggestive definition turns out to be useful:

Definition 3 *For any object (ρ, γ) let $|i\rangle$ and $|j\rangle$ be eigenvectors of γ. Let E_i and E_j be the corresponding eigenvalues of the system's Hamiltonian, i.e.,*

$$E_j - E_i = \frac{(\ln\langle i|\gamma|i\rangle - \ln\langle j|\gamma|j\rangle)}{\beta}.$$

Then the **relative inverse temperature** *with respect to the states $|i\rangle$ and $|j\rangle$ is defined to be*

$$\beta_{|i\rangle,|j\rangle} := \frac{\ln\langle i|\rho|i\rangle - \ln\langle j|\rho|j\rangle}{E_j - E_i}.$$

Similarly, we define the relative temperature

$$T_{|i\rangle,|j\rangle} := \frac{1}{k\beta_{|i\rangle,|j\rangle}}.$$

Using this definition we have an easy criterion for the possibility of cooling:

Theorem 1 *An object $O := (\rho, \gamma)$ can be used for cooling a qubit $Q := (\sigma, \sigma)$ with energy gap E and the inverse temperature β if and only if there is a pair $|i\rangle$ and $|j\rangle$ of eigenvectors of the Hamiltonian H (corresponding to γ) with different eigenvalues E_i and E_j such that $E_i - E_j = E$ and*

$$\beta_{|i\rangle,|j\rangle} > \beta.$$

Proof: Assume $\beta_{|i\rangle,|j\rangle} > \beta$. Let $|1\rangle, \ldots, |l\rangle$ be a basis of eigenvectors of γ. Let $|0\rangle$ and $1\rangle$ be the lower and upper state of the two-level system (In case of degenerated levels the choice is irrelevant). Then the occupation probability for the ground state is given by

$$\langle 0|\sigma|0\rangle = \sum_j \langle j|\rho|j\rangle\langle 0|\sigma|0\rangle.$$

Now we perform the transformation u by permuting the states by the involution

$$|i\rangle \otimes |0\rangle \quad \leftrightarrow \quad |j\rangle \otimes |1\rangle$$

and acting trivial on the other tensor product basis states. The probability for the lower state is changed by the amount

$$\begin{aligned} &tr((u(\rho \otimes \sigma)u^* - (\rho \otimes \sigma))(1 \otimes |0\rangle\langle 0|)) \\ &= \langle j|\rho|j\rangle\langle 1|\sigma|1\rangle - \langle i|\rho|i\rangle\langle 0|\sigma|0\rangle. \end{aligned}$$

The latter term is negative by assumption and due to the definition of β and $\beta_{|i\rangle,|j\rangle}$.

Assume $\beta_{|i\rangle,|j\rangle} \leq \beta$. Clearly, for any j the spectral projection P_j can be written as

$$P_j = (Q_+ \otimes |0\rangle\langle 0|) \oplus (Q_- \otimes |1\rangle\langle 1|),$$

where Q_+ and Q_- are spectral projections of γ. Since σ commutes with $|0\rangle\langle 0|$ and $|1\rangle\langle 1|$ we have:

$$\begin{aligned} P_j(\rho \otimes \sigma)P_j = &Q_+\rho Q_+ \otimes |0\rangle\langle 0|\langle 0|\sigma|0\rangle \oplus \\ &Q_-\rho Q_- \otimes |1\rangle\langle 1|\langle 1|\sigma|1\rangle. \end{aligned}$$

The eigenvalues of the first component in this direct sum belong to Γ^j_+, those in the second to Γ^j_-. If $E_i - E_j = E$ the quotient of any eigenvalues of $Q_+\rho Q_+$ and any eigenvalue of $Q_-\rho Q_-$ can never exceed $e^{-\beta_{|i\rangle,|j\rangle}E}$. Therefore $\beta_{|i\rangle,|j\rangle} \leq \beta$ implies that condition (2) in Lemma 1 is fulfilled. □

In the sense of the definition 3 we have the strong statement, that the low temperature which *should be attained* in the qubit must already be *inherent in the used resources*. For the moment, the problem of cooling seems to be circular and one might ask, why cooling is possible at all.

We will show that there is an easy answer, since arbitrary low relative temperatures can be obtained by composing *many* objects deviating from their equilibrium state. In particular, the composition of two objects O_1 and O_2 being in their thermal equilibrium states for the inverse temperature β_1 and β_2, respectively can contain

inverse temperatures larger than β_1 and β_2. This is the quantum analogue of the well-known fact from classical thermodynamics, that *cooling* can be driven by *heat* without any other energy supply. This principle is used in an absorption heat pump for instance.

This indicates that the calculation of the relative temperatures obtained by *composing* objects might give interesting insights in the problem of 'the origin of low temperatures'. We will develop a quite general theory of relative temperatures in composed systems, but we will restrict our investigations to the case that the density matrices of the considered systems are diagonal with repect to any basis diagonalizing the Hamiltonian. Furthermore we will restrict the class of allowed transformations to those which permute the basis states. We will call this the 'quasi-classical case' and define:

Definition 4

1. *A* **quasi-classical (l-level) system** *is described by a vector $g \in \mathbb{R}^l$ defining the probabilities for finding the system in one of the states $\{1, \ldots, l\}$.*
2. *A* **quasi-classical object** *is a pair (p, g) where $p \in \mathbb{R}^l$ is the probability distribution of the actual state and $g \in \mathbb{R}^l$ the equilibrium distribution. Let p_i and g_i be the components of the vectors p, g.*
3. *An* **allowed transformation** *is a permutation π of the states $1, \ldots, l$ which leaves g invariant, i.e., $g_{\pi(i)} = g_i$ for every $1 \leq i \leq l$.*
4. *Composition of objects and composition and restriction of systems are defined as in the quantum case (see Definition 1), i.e., we have tensor product vectors describing joint probability distributions, restrictions of objects are defined by marginal distributions.*

   In analogy to Definition 3, a relative inverse temperature $\beta_{i,j}$ can be assigned to any pair $(i, j) \in \{1, \ldots, l\}^2$.

Now we are able to give an example for the statement that the composition of an n-fold copy of the identical object can lead to arbitrary low temperatures as n increases: Take a system with the energy levels $0, E, 2E$ being in the statistical state $p = (p_1, p_2, p_3)$. Let n be an odd number and set $n = 2l - 1$. We assume

$$1 > \frac{p_3}{p_2}\frac{p_1}{p_2} =: d$$

In the n-fold composition of the object (p, g), i.e., in $(p^{\otimes n}, g^{\otimes n})$, we consider the following two states $|1\rangle$ and $|2\rangle$:

Let $|1\rangle$ be some state in which l of the subsystems are on the level $2E$ and $l - 1$ are in the level 0. Let $|2\rangle$ be the unique state where every system has energy E. The quotient of the probabilities of these two states is

$$d^l \frac{p_2}{p_1},$$

the energy difference of both is E. Hence we get the relative inverse temperature

$$\beta_{1,2} = -\frac{1}{E}(l \ln d + \ln(p_2/p_1)),$$

which tends to infinity for increasing l.

It turns out, that the problem of determining the relative inverse temperatures in an object composed of two quasi-classical ones is a geometrical one: For any pair (i, j) of states of the object $O := (p, g)$ we define a vector $v_{i,j} \in \mathbb{R}^2$ by

$$v_{i,j}(O) := (\frac{1}{\beta} \ln(g_i/g_j), \ln(p_i/p_j)). \tag{1}$$

Note that the quotient of relative inverse temperature and the reference inverse temperature β of the pair (i, j) is given by the tangens of the angle enclosed by v_{ij} and the x-axis. In any composed object $O \times \tilde{O}$ we denote the state $(i, \tilde{i})$ by 1 and the state $(j, \tilde{j})$ by 2. We obtain

$$v_{1,2}(O \times \tilde{O}) = v_{i,j}(O) + v_{\tilde{i},\tilde{j}}(\tilde{O})$$

as the sum of the corresponding vectors for the subsystems.

If we define $V_O := \{v_{i,j}(O) | 1 \leq i, j \leq l\}$, we get: The inverse temperatures available in the n-fold of the object are given by the possible values of $\tan \phi$, where ϕ is the angle enclosed by the vector

$$\sum_{i=1}^{n} x_i$$

and the x-axis and x_i are arbitrary vectors taken from the set V_O.

Therefore the problem of finding the lowest relative temperature in a composed object is a geometrical one.

IV. INCLUDING THE ENVIRONMENT

The problem of finding the lowest relative temperature in a given object is a little bit artificial for two reasons: Firstly, the optimal pair of states can only be used for cooling those two-level systems which have the same energy gap. Of course it would be more natural to fix the required energy gap in advance. But then, in the generic case, one will not find any appropriate pair of states at all. Secondly, it does not make sense to assume that the two-level system and the resources must be isolated from the rest of the world. Since it is even impossible to *prevent* this systems from interacting with the rest of the world, it seems unphysical to *forbid* such an interaction even if it would *help* for cooling.

In a modified model, both shortcomings of the theory can be removed at once: We will investigate the possibilities of cooling a given object under the assumption that one can use the help of arbitrary additional equilibrium objects. They can be thought of as the system's environment, i.e., physical systems as particles and field surrounding the considered objects. We will assume the environment to be in its equilibrium state, since we consider this as its *defining* property: every non-equilibrium object would be reckoned as additional *resources*.

In other words, we will investigate the 'worth' of the resources with respect to cooling under the assumption that *equilibrium* objects can be obtained *for free*. There are two reasons why the inclusion of ancilla equilibrium objects may help for cooling: On the one hand, generically the energy gaps of the resources pure states will not coincide with the energy difference of the two-level system. Then, an additional equilibrium object with an appropriate level structure enables to perform nontrivial transformations at all. On the other hand, a *cooling* process driven by *heat* without any other energy supply is only possible with the use of objects having the (lower) reference temperature. Loosely speaking: The Second Law states that 'heat without cold is worthless' for driving any process.

In order to avoid unnecessary mathematical complications, we will assume the ancilla objects to be *finite* dimensional quantum systems. This should not be considered as an essential restriction, since we are only interested in statements which do not refer to any particular level structure of the ancillas. Furthermore, in some sense the infinite dimensional case is included in our analysis, since we allow sequences of systems with growing dimension as environments.

We shall see that the help of an appropriate environment is so useful, that in the quasi-classical case even *every* non-equilibrium object enables cooling. For the quantum case we will show, that an object enables cooling if and only if the *time average* of its state differs from the equilibrium state. The time average $\overline{\rho}$ is defined by

$$\overline{\rho} := \lim_{t\to\infty} \frac{1}{t}\int_0^t e^{-iHs}\rho e^{iHs} ds.$$

It is given by

$$\overline{\rho} = \sum_j P_j \rho P_j$$

where P_j are the spectral projections of the system's Hamiltonian H (and the corresponding equilibrium state γ). This can be seen by theorems from ergodic theory on Hilbert spaces [15]: By taking the trace as an inner product on the space of matrices, the time evolution is unitary on the density matrices and the map $\rho \mapsto \sum P_j \rho P_j$ is the orthogonal projection on the eigenspace of the generator $i[H,.]$ with eigenvalue 0.

If an object enables cooling of a qubit having environment's temperature, it is natural to ask whether the object allows cooling even if the qubit is already colder than the environment.

We define the *lower* (respectively upper) *limit temperature* of a resource object as the greatest (respectively lowest) initial temperature of the qubit such that cooling (respectively heating) is just impossible. Note that the reference temperature, i.e., the temperature of the used ancilla objects, is fixed however. We will introduce a parameter which will turn out to determine the lower and the upper limit temperatures at once:

Definition 5 *For any object $O := (\rho, \gamma)$ and any pair $|i\rangle$, $|j\rangle$ of eigenstates of γ with eigenvalues λ_i, λ_j we set:*

$$f_{|i\rangle,|j\rangle}(O) := \ln\langle i|\rho|i\rangle - \ln\langle j|\rho|j\rangle - \ln\lambda_i + \ln\lambda_j.$$

Then we define the maximal diagonal deviation *from equilibrium as*

$$D(O) := \max\{|f_{|i\rangle,|j\rangle}|\}, \tag{2}$$

where the maximum is taken over all pairs of eigenstates.

Obviously $D(O) = 0$ if and only if the diagonal entries of ρ agree with the entries of the equilibrium state with respect to every basis diagonalizing γ. This justifies the terminology. Easy considerations show, that $D((\rho,\gamma)) = 0$ if and only if $\overline{\rho} = \gamma$, where $\overline{\rho}$ is the time average of ρ. Furthermore we have the following reformulation of Definition 5:

Lemma 2 *Let $O := (\rho, \gamma)$ be an arbitrary object and P_i be the spectral projections of γ for the eigenvalues λ_i. Then the maximal diagonal deviation is given by:*

$$D(O) = \max_{i,j}\{|\ln(\|P_i\rho P_i\|) + \ln(\|(P_j\rho P_j)^{-1}\|) - \ln\lambda_i + \ln\lambda_j|\},$$

where $(.)^{-1}$ denotes the pseudoinverse of any matrix and $\|.\|$ is the operator norm defined by $\|a\| := \max_x\{\|ax\|/\|x\|\}$ where $\|x\|$ is the euclidean norm of the vector x.

Proof: Obviously, Definition 5 can be reformulated as

$$D(O) = \max_{i,j}\max_{|\psi\rangle,|\phi\rangle}\{|\ln(\langle\psi|\rho|\psi\rangle) - \ln(\langle\phi|\rho|\phi\rangle) - \ln\lambda_i + \ln\lambda_j|\},$$

where $|\psi\rangle$ and $|\phi\rangle$ have to be eigenvectors of γ corresponding to λ_i and λ_j, respectively. The term in the braces is maximized if $|\psi\rangle$ is the eigenvector of $P_i\rho P_i$ corresponding to its largest eigenvalue and $|\phi\rangle$ corresponding to the smallest eigenvalue of $P_j\rho P_j$. But then one has:

$$\langle\psi|\rho|\psi\rangle = \|P_i\rho P_i\|$$

and

$$\langle\phi|\rho|\phi\rangle = \|(P_j\rho P_j)^{-1}\|^{-1}.$$

□

The maximal diagonal deviation is a superadditive quantity, for quasi-classical objects it is only additive:

Theorem 2 *We have*

$$D(O \times \tilde{O}) \geq D(O) + D(\tilde{O})$$

for arbitrary objects $O := (\rho, \gamma)$ *and* $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ *with equality if*[2] ρ *commutes with* γ or $\tilde{\rho}$ *commutes with* $\tilde{\gamma}$.

Proof: For the object O let $|i\rangle$ and $|j\rangle$ a pair of eigenvectors of γ maximizing the expression (2) and for the object $\tilde{O}$ let $|l\rangle$ and $|k\rangle$ be such a maximizing pair of eigenvectors of $\tilde{\gamma}$. Then we have

$$f_{|i\rangle\otimes|l\rangle,|j\rangle\otimes|k\rangle} = f_{|i\rangle,|j\rangle} + f_{|l\rangle,|k\rangle}.$$

In case that the signs of the two terms on the right hand side do not agree, we can change it by exchanging $|l\rangle$ and $|k\rangle$ due to the antisymmetry of f.

Assume that ρ commutes with γ. Let Q_i be the spectral projections of $\gamma \otimes \tilde{\gamma}$ with the corresponding eigenvalues μ_i. Write Q_i as

$$Q_i = \oplus_l (P_l^i \otimes \tilde{P}_l^i)$$

where P_l^i and $\tilde{P}_l^i$ are spectral projections of γ and $\tilde{\gamma}$ with eigenvalues λ_l^i and $\tilde{\lambda}_l^i$ (respectively) such that $\lambda_l^i \tilde{\lambda}_l^i = \mu_i$. For any matrix let a denote its pseudoinverse by a^{-1}. Due to Lemma 2 the maximal diagonal deviation can be written in the form

$$\begin{aligned} &D(O \times \tilde{O}) = \\ &\max_{i,j} \Big\{ |\ln \|Q_i(\rho \otimes \tilde{\rho})Q_i\| + \ln \|(Q_j(\rho \otimes \tilde{\rho})Q_j)^{-1}\| \\ &\qquad - \ln(\mu_i) + \ln(\mu_j)| \Big\}. \end{aligned}$$

From $[\rho, \gamma] = 0$ we conclude $P_l^i \rho P_m^i = 0$ for $l \neq m$. Hence we have:

$$\begin{aligned} D(O \times \tilde{O}) &= \max_{i,j} \Big\{ |\ln \| \oplus_l ((P_l^i \rho P_l^i) \otimes (\tilde{P}_l^i \tilde{\rho} \tilde{P}_l^i))\| \\ &\quad + \ln \| \oplus_l ((P_l^j \rho P_l^j)^{-1} \otimes (\tilde{P}_l^j \tilde{\rho} \tilde{P}_l^j)^{-1})\| \\ &\quad - \ln \mu_i + \ln \mu_j| \Big\} \\ &= \max_{i,j} \Big\{ |\ln \max_l \|(P_l^i \rho P_l^i) \otimes (\tilde{P}_l^i \tilde{\rho} \tilde{P}_l^i)\| \\ &\quad + \ln \max_l \|(P_l^j \rho P_l^j)^{-1} \otimes (\tilde{P}_l^j \tilde{\rho} \tilde{P}_l^j)^{-1}\| \\ &\quad - \ln \mu_i + \ln \mu_j| \Big\} \\ &\leq D(O) + D(\tilde{O}) \end{aligned}$$

□

Since the maximal diagonal deviation vanishes for every equilibrium object we have:

Corollary 1 *The maximum diagonal deviation is stable with respect to a composition with arbitrary systems in its equilibrium state, i.e. we have*

$$D(O \times O_e) = D(O)$$

for every object O *and every equilibrium object* $O_e := (\tilde{\gamma}, \tilde{\gamma})$.

Despite the fact, that the quantity D is not additive in general, its asymptotical increase for composition of a large number n of identical objects is of the order n:

Lemma 3 *Let* O *be an arbitrary object. Then*

$$\lim_{n\to\infty} \frac{D(O^n)}{n}$$

exists.

Proof: Set $O := (\rho, \gamma)$ and $f(n) := D(O^n)$. Firstly we show that the sequence $f(n)/n$ is bounded from above: Due to Lemma 2 and the triangle inequality one has

$$\begin{aligned} D(O^n) &\leq |\ln \|\rho^{\otimes n}\|| + |\ln \|\rho^{-n}\|| \\ &\quad + |\ln \|\gamma^{\otimes n}\|| + |\ln \|\gamma^{-n}\|| \\ &= n(|\ln \|\rho\|| + |\ln \|\rho\|| + |\ln \|\gamma\|| + |\ln \|\gamma\||) \end{aligned}$$

Due to the superadditivity of D one concludes

$$f(lm + r) \geq l f(m) + f(r) \ \ \forall m, l, r \in \mathbb{N}.$$

Now let m be fixed. For any n define $l_n := \lfloor (n/m) \rfloor$ and $r_n := n - m\, l_n$, hence $n = l_n\, m + r_n$, where $\lfloor . \rfloor$ denotes the integer part of a real number. We have

$$\frac{f(n)}{n} = \frac{f(l_n\, m + r_n)}{l_n\, m + r_n} \geq \frac{l_n\, f(m) + f(r_n)}{l_n\, m + r_n}.$$

Since the right hand term tends to $f(m)/m$ for $n \to \infty$, we conclude, that no accumulation point of $f(n)/n$ can be smaller than $f(m)/m$. Because m is arbitrary, $f(n)/n$ can have only one cumulation point. □

The maximal diagonal deviation can be interpreted geometrically: For any pair $|i\rangle$ and $|j\rangle$ of states set

$$p_i := \langle i|\rho|i\rangle \ \text{ and } \ p_j := \langle j|\rho|j\rangle. \tag{3}$$

Then we consider the vector

$$v_{i,j}(O)$$

defined as in equation (1) and note, that D is given by maximizing the length of the projection of the vector $v_{i,j}(O)$ on the straight line $y = -x/\beta$.

The quantity $D(O)$ shows an interesting symmetry which will turn out to be important in the theory of heating and cooling. This can be seen by the introducing the following terminology:

[2]There are easy examples, showing that this condition cannot be dropped: Take a qubit with $diag(0, E)$ as Hamiltonian and a coherent superposition of $|0\rangle$ and $|1\rangle$ such that the diagonal entries of the corresponding density matrix agree with the equilibrium distribution. Hence D vanishes for this object. But the composition of two such objects has non-vanishing D.

Definition 6 *For any inverse temperature β_1 we call*

$$\beta_2 := 2\beta - \beta_1$$

its **complementary inverse temperature** *relative to the reference temperature β.*

One checks easily that two qubits (with the same energy gap) having inverse temperatures β_1 and β_2 have the same maximal diagonal deviation from their equilibrium state. Furthermore we find that for any temperature, its complementary value is available by coupling the considered system to an equilibrium object:

Assume we have a pair $|i\rangle$ and $|j\rangle$ of eigenstates of the Hamiltonian with relative inverse temperature $\beta_{|i\rangle,|j\rangle}$. Take a qubit with energy difference $E := 2(E_i - E_j)$ with inverse temperature β. Then we find

$$\beta_{|i\rangle\otimes|0\rangle,|j\rangle\otimes|1\rangle} = 2\beta - \beta_{|i\rangle,|j\rangle},$$

i.e., the complementary temperature is available for a pair of states with the same energy gap as the original one.

As a consequence we see, that if very high relative temperatures are inherent in an object, then very low temperatures are inherent in the composition with an equilibrium object. Furthermore, lower and upper limit temperatures of any object O are determined by $D(O)$. In order to state this more precisely we define:

Definition 2 (new) *Let Q be a qubit in any diagonal state. Let O be an arbitrary object. We say, O can be used for cooling or heating Q, respectively, if there is an equilibrium object O_e such that there is an allowed transformation on $O \times O_e \times Q$ decreasing the occupation probability for the upper or lower state, respectively.*

From now on we will use this terminology (in contrast to Definition 2) and obtain:

Theorem 3 *Let Q be a qubit in any diagonal state. An object O can be used for cooling* and *heating Q if and only if*

$$D(O) > D(Q).$$

In the case that

$$D(O) \leq D(Q)$$

the resource O is **worthless** *in the sense, that it can only be used for cooling if Q is hotter than the equilibrium state and it can be used for heating if Q is colder than the equilibrium state.*

Proof: Let $Q := (diag(s,r), diag(t,v))$, where r is the occupation probability for the upper state. Following Theorem 1 we know that $O \times O_e$ can be used for cooling if and only if there is a pair of states $|i\rangle$ and $|j\rangle$ in the composed system such that

$$p_i/p_j < r/s,$$

where we have taken the abbreviations given by equation (3) and $E_i - E_j = E$ if E_i, E_j are the corresponding energies and $E > 0$ is the energy gap of the qubit. Assume the qubit to be colder than the environment. Then

$$-D(Q) = \ln(r/s) + \beta E.$$

By definition of D we have

$$-D(O \times O_e) + \beta E \leq \ln(p_i/p_j) \leq D(O \times O_e) + \beta E.$$

Assume $D(O) \leq D(Q)$. Using $D(O \times O_e) = D(O)$ and equation (2) one concludes

$$\ln(r/s) \leq \ln(p_i/p_j),$$

hence cooling is impossible. Hence we see, that $D(O) > D(Q)$ is necessary for cooling an already cold qubit. Similarly one shows, that this condition is necessary for heating a hot one.

Assume $D(O) > D(Q)$. Choose a pair of states $|i\rangle$ and $|j\rangle$ of the object O such that

$$D(O) = |\ln(p_i/p_j) + \beta(E_i - E_j)|.$$

Due to the antisymmetry of the right hand term with respect to i and j we can even assume

$$D(O) = \ln(p_i/p_j) + \beta(E_i - E_j)$$

without loss of generality. By definition of $D(Q)$ we have

$$\ln(p_i/p_j) + \beta(E_i - E_j) > |\ln(r/s) + \beta E|.$$

We conclude

$$\ln(p_i/p_j) + \beta(E_i - E_j) > -\ln(r/s) - \beta E$$

and

$$\frac{\ln(p_i/p_j) + \beta(E_i - E_j + E)}{E} > \frac{-\ln(r/s)}{E}.$$

Now we take an ancilla qubit with the energies $\tilde{E} := E_i - E_j + E$ and 0 for the states $|1\rangle$ and $|0\rangle$. Note that here $|1\rangle$ need not be the upper state since we do not assume $\tilde{E} > 0$. In the composition of O with the ancilla qubit the pair of states

$$|i\rangle \otimes |1\rangle \quad \text{and} \quad |j\rangle \otimes |0\rangle$$

have the energy gap E and for the relative inverse temperature of this pair we conclude:

$$\beta_{|i\rangle\otimes|1\rangle,|j\rangle\otimes|0\rangle} = \frac{\ln(p_i/p_j) + \beta(E_i - E_j + E)}{E} > \frac{-\ln(r/s)}{E}.$$

Hence this pair can be taken for cooling due to Theorem 1. In a similar way one can conclude that the object O can serve for heating. □

The statement of Theorem 3 can be reformulated as follows: The lower and upper limit temperatures of an object O are given by the temperatures of the two diagonal states $\rho_{1,2} := diag(s_{1,2}, r_{1,2})$ of the qubit $Q := (diag(s_{1,2}, r_{1,2}), diag(t, v))$ with the property $D(Q) = D(O)$.

To avoid false conclusions at this point we emphasize that in general a *single* copy of an object O is not sufficient for cooling or heating the qubit down or up to the limit temperatures if the latter has the reference temperature initially. The limit temperatures can only be approached by running an infinite number of stages of the same cooling or heating procedure. This requires an infinite number of copies of the object O since the resource has to be refreshed in each stage.

This observation leads to another natural question: Given any object O, what is the lowest temperature of the qubit which can be prepared by using one single copy of the resource O if the initial state of the qubit has the reference temperature. One can formulate this problem more generally: Assume we have an object O and any other system being in its equilibrium state $\tilde{\gamma}$ initially. Which states $\tilde{\gamma}$ of the latter system can be prepared by coupling it to the object O and arbitrary ancilla equilibrium objects? With other words: Which objects $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ can be obtained with the help of the resources O? This leads straightforwardly to a relation which is like a quasi-ordering on the set of objects, which we shall call the *conversion order*:

Definition 7 *We say 'the object $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ can be obtained by using the resource $O := (\rho, \gamma)$', formally written as*

$$O \geq \tilde{O},$$

if there exists a sequence of equilibrium objects $O_{e,n} := (\hat{\gamma}_n, \hat{\gamma}_n)$ and a sequence of allowed transformations u_n on

$$O \times O_{e,n} \times \tilde{O}$$

such that

$$\lim_{n\to\infty} tr_{12}(u_n(\rho \otimes \hat{\gamma}_n \otimes \tilde{\gamma})u_n^*) = \tilde{\rho},$$

where tr_{12} denotes the partial trace over the left most and the middle component in the tensor product.

It is easy to give the following necessary condition for $O \geq \tilde{O}$:

Theorem 4 *Let $\mathcal{H}$ and $\tilde{\mathcal{H}}$ be the Hilbert spaces corresponding to the objects $O := (\rho, \gamma)$ and $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$, respectively. If $O \geq \tilde{O}$ then there is a completely positive trace preserving map G from the set of density matrices on $\mathcal{H}$ to the set of density matrices on $\tilde{\mathcal{H}}$ satisfying*

$$G\rho = \tilde{\rho} \quad and \quad G\gamma = \tilde{\gamma} \tag{4}$$

as well as the covariance condition

$$[\tilde{H}, G(.)] = G([H, .]), \tag{5}$$

where H and $\tilde{H}$ are Hamiltonians corresponding to the equilibrium states γ and $\tilde{\gamma}$, respectively.

Proof: For every equilibrium object $O_{e,n} := (\hat{\gamma}_n, \hat{\gamma}_n)$ and every allowed transformation u_n on $O \times O_{e,n} \times \tilde{O}$ we define

$$G_n(\sigma) := tr_{12}(u_n(\sigma \otimes \hat{\gamma}_n \otimes \tilde{\gamma})u_n^*)$$

for every density matrix σ on $\mathcal{H}$. Every G_n is a completely positive trace preserving map satisfying $G_n(\gamma) = \tilde{\gamma}$ since conjugation by u_n preserves the equilibrium state of the total system. Since the set of completely positive trace preserving maps for given spaces $\mathcal{H}$ and $\tilde{\mathcal{H}}$ is compact, the sequence G_n has a convergent subsequence. Let G denote its limit point. Obviously we have $G(\rho) = \tilde{\rho}$ and $G(\gamma) = \tilde{\gamma}$. The covariance condition $[\tilde{H}, G(.)] = G([H, .])$ follows easily from the fact that the allowed transformation commutes with the free evolution of the total system and preserves the equilibrium states in every tensor component. □

In the following we will try to work out the conversion order as explicitly as possible. We start by doing this for quasi-classical objects. In this case the quasi-ordering can be given explicitly:

Theorem 5 *Let $O := (p, g)$ and $\tilde{O} := (\tilde{p}, \tilde{g})$ be quasi-classical objects. Then*

$$O \geq \tilde{O}$$

if and only if there is a stochastic matrix A such that

$$Ap = \tilde{p} \quad and \quad Ag = \tilde{g}. \tag{6}$$

Proof: Assume $O \geq \tilde{O}$. Let $\rho, \gamma, \tilde{\rho}, \tilde{\gamma}$ be the density matrices with diagonal entries $p, g, \tilde{p}$, and $\tilde{g}$, respectively. Assume $p, g \in \mathbb{R}^l$ and $\tilde{p}, \tilde{g} \in \mathbb{R}^{\tilde{l}}$. For any density matrix σ acting on $\mathbb{C}^{\tilde{l}}$ we define the vector $q(\sigma) \in \mathbb{R}^{\tilde{l}}$ by the diagonal of σ. For every $i \leq l$ define the density matrix

$$e_i := diag(0, \ldots, 0, 1, 0, \ldots, 0)$$

where the entry '1' is on position i. Define a stochastic $\tilde{l} \times l$-matrix A by

$$Ar = q(G(\sum_i r_i e_i)),$$

where r_i is the i-th component of an arbitrary vector $r \in \mathbb{R}^l$. Obviously, both equations in (6) are fulfilled.

Assume there is a stochastic matrix A such that $Ap = \tilde{p}$ and $Ag = \tilde{g}$.

For every $n \in \mathbb{N}$ choose the environment

$$O_{e,n} := (g^{\otimes n} \otimes \tilde{g}^{\otimes n}, g^{\otimes n} \otimes \tilde{g}^{\otimes n}).$$

Assume $p \in \mathbb{R}^l$ and $\tilde{p} \in \mathbb{R}^{\tilde{l}}$. Hence the pure states of the systems described by g and $\tilde{g}$ can be named by the symbols $1, \ldots, l$ and the symbols $1, \ldots, \tilde{l}$, respectively.

Let $\mathcal{S}_n$ be the set of pure states in the composed system described by the equilibrium state

$$g \otimes g^{\otimes n} \otimes \tilde{g}^{\otimes n} \otimes \tilde{g}.$$

Every element of $\mathcal{S}_n$ is characterized by a word of length $n+1$ over the alphabet $\{1, \ldots, l\}$ and a word of length $n+1$ over the alphabet $\{1, \ldots, \tilde{l}\}$. In the following, only four attributes of these word pairs are relevant:

1. the first symbol of the first word, denoted by j.
2. the numbers of occurrences of the symbols $1, \ldots, l$ in the first word, denoted by $r_1, \ldots, r_l$, or simply by the vector $r \in \mathbb{N}^l$ with $\sum_i r_i = n+1$.
3. the numbers of occurrences of symbols $1, \ldots, \tilde{l}$ in the second word, denoted by $s_1, \ldots, s_{\tilde{l}}$ or the vector $s \in \mathbb{N}^{\tilde{l}}$ with $\sum_i s_i = n+1$.
4. the last symbol of the second word, denoted by x.

Hence we assign the 4-tuple (j, r, s, x) to every pair of words. Now let n, r, s be fixed. Note that all the states with a common vector r and s have the same energy. We write $\{(j, r, s, .)\}$ for the cylindric set of states having j, r, s as the first three attributes. Their numbers of elements are given by a product of two multinomial coefficients

$$b_j := \frac{r_j \; n!}{\prod_{i \le l}(r_i)!} \frac{(n+1)!}{\prod_{i \le \tilde{l}}(s_i)!} \tag{7}$$

Accordingly, write $\{(., r, s, x)\}$ for the set of states with r, s, x as the last three attributes. Their numbers of elements are given by

$$c_x := \frac{(n+1)!}{\prod_{i \le l}(r_i)!} \frac{s_x \; n!}{\prod_{i \le \tilde{l}}(s_i)!} \tag{8}$$

Note that these sets depend on the number n, i.e., the size of the environment, although we do not indicate this explicitly by indices.

Let a_{xj} with $j \le l, x \le \tilde{l}$ be the entries of the matrix A. Now we define for each x the l numbers

$$m_{xj} := \min\{c_x - \sum_{i<j} m_{xi}, \lfloor a_{xj} b_j \rfloor\},$$

where $\lfloor . \rfloor$ denotes the integer part of a real number.

For each j choose $\tilde{l}$ disjoint sets $M_{xj} \subset \{(j, r, s, .)\}$ with m_{xj} elements. This is possible since

$$\sum_x m_{xj} \le \sum_x a_{xj} b_j = b_j.$$

Note that we do not indicate explicitly that the numbers b_j, c_x, m_{xj} as well as the sets M_{xj} depend on (r, s). Choose an injective map

$$\hat{\pi}_{r,s} : \cup_{x,j} M_{xj} \to \{(., r, s, .)\}$$

such that

$$\hat{\pi}_{r,s}(M_{xj}) \subset \{(., r, s, x)\}.$$

This is possible since $\sum_j m_{xj} \le c_x$. Extend $\hat{\pi}_{r,s}$ to a bijection

$$\pi_{r,s} : \{(., r, s, .)\} \to \{(., r, s, .)\}.$$

Now perform such a transformation $\pi_{r,s}$ on every set $\{(., r, s, .)\} \subset \mathcal{S}_n$. For every n, this defines a bijection

$$\pi_n : \mathcal{S}_n \to \mathcal{S}_n.$$

Let P_n be the probability measure on $\mathcal{S}_n$ defined by the composed system's initial state

$$p \otimes g^{\otimes n} \otimes \tilde{g}^{\otimes n} \otimes \tilde{g}.$$

Let $\tilde{P}_n$ be the image of P_n under the transformation π_n, i.e.,

$$\tilde{P}_n := P_n \circ \pi_n^{-1}.$$

Let $\mathcal{T}_n \subset \{(r, s) \in \mathbb{N}^l \times \mathbb{N}^{\tilde{l}} \mid \sum r_i = n+1, \; \sum s_i = n+1\}$ be a such that

$$\lim_{n \to \infty} \sum_{(r,s) \in \mathcal{T}_n} \tilde{P}_n(\{(., r, s, .)\}) =$$
$$\lim_{n \to \infty} \sum_{(r,s) \in \mathcal{T}_n} P_n(\{(., r, s, .)\} = 1$$

and

$$\lim_{n \to \infty} \max_{(r,s) \in \mathcal{T}_n} \{\|\frac{r}{n} - g\| + \|\frac{s}{n} - \tilde{g}\|\} = 0.$$

This is possible due to the law of large numbers, since the words with

$$\|\frac{r}{n} - g\| \approx 0 \;\text{ and }\; \|\frac{s}{n} - \tilde{g}\| \approx 0$$

are *typical* (c.f. [16]).

Now we have to show, that asymptotically the probabilities of the symbols $1, \ldots, \tilde{l}$ in the right most component of the system are changed from $\tilde{g}_1, \ldots, \tilde{g}_{\tilde{l}}$ to $\tilde{p}_1, \ldots, \tilde{p}_{\tilde{l}}$ by the permutations π_n, i.e., we must show

$$\sum_{r,s} \tilde{P}_n(\{(., r, s, x)\}) \to \tilde{p}_x.$$

We do this by proving

$$\max_{(r,s) \in \mathcal{T}_n} |\frac{\tilde{P}_n(\{(., r, s, x)\})}{\tilde{P}_n(\{(., r, s, v)\})} - \frac{\tilde{p}_x}{\tilde{p}_v}| \to 0.$$

With respect to the initial probability measure P_n every word pair with attributes (j,r,s,x) has the probability

$$w_j := \frac{p_j}{g_j} \prod_{i \leq l} g_i^{r_i} \prod_{i \leq \tilde{l}} \tilde{g}_i^{s_i}. \tag{9}$$

If for every n our attention is only restricted to those vector pairs (r,s) which are elements of $\mathcal{T}_n$, we have the following asymptotic statements as n goes to infinity:

1. The quotients c_x/b_j tend to $\tilde{g}_x/g_j$ and b_j/b_i tend to g_j/g_i due to equations (7) and (8).

2. Therefore $m_{xj}/b_j \to a_{xj}$. This follows from 1 by induction over j because $\sum_j a_{xj} g_j = \tilde{g}_x$.

3. The set $\{(j,r,s,.)\}$ is more and more exhausted by $\cup_x M_{xj}$ in the sense that the number of elements of its complement becomes negligible compared to the number of elements of $\{(j,r,s,.)\}$. This shows that the total probability of the complement becomes irrelevant, since all its elements have the same probability.

We conclude:

$$\begin{aligned} &\lim_{n\to\infty} \max_{(r,s)\in\mathcal{T}_n} \frac{\tilde{P}_n(\{(.,r,s,x)\})}{\tilde{P}_n(\{(.,r,s,v)\})} \\ &= \lim_{n\to\infty} \max_{(r,s)\in\mathcal{T}_n} \frac{\sum_j m_{xj} w_j}{\sum_j m_{vj} w_j} \\ &= \frac{\sum_j a_{xj} g_j w_j}{\sum_j a_{vj} g_j w_j} = \frac{\sum_j a_{xj} p_j}{\sum_x a_{vj} p_j} = \frac{\tilde{p}_x}{\tilde{p}_v}. \end{aligned}$$

For reasons of convenience we dropped the index n for r, s, m_{xj}, b_j.

The reason for the first equality is given by statement 3. The second one is proven by the statements 1 and 2. The third equality is due to equation (9) and the last one by assumption.

The statements 1-3 reflect the following idea behind our construction: The part a_{xj} of the elements in $\{(j,r,s,.)\}$ is mapped onto an element in $\{(.,r,s,x)\}$. Since the ratios of the sizes of these sets behave asymptotically as $g_j : \tilde{g}_x$, the condition $\sum_j a_{xj} g_j = \tilde{g}_x$ guarantees that such a map can be constructed as a bijective one. For typical (r,s), the numbers of elements in $\{(1,r,s,.)\}, \ldots, \{(l,r,s,.)\}$ are related to each other by $g_1, \ldots, g_l$ and the probabilities of single elements in $\{(1,r,s,.)\}, \ldots, \{(l,r,s,.)\}$ are related by $p_1/g_1, \ldots, p_l/g_l$. The total probability of the set $\{(.,.,.,x)\}$ after having performed the transformation is therefore given by $\sum_j a_{xj} g_j p_j/g_j = \sum_j a_{xj} p_j = \tilde{p}_x$. □

Loosely speaking, we have shown, that any stochastic matrix, which maps an equilibrium state of the first system on the equilibrium state of the second one, can be carried out by an energy conserving process provided that any ancilla system being in its equilibrium state can be used.

Note that Theorem 5 shows a symmetry with respect to an exchange of the actual probability distribution p and the equilibrium distribution g:

Corollary 2 *We have:*

$$(p,g) \geq (\tilde{p},\tilde{g})$$

if and only if

$$(g,p) \geq (\tilde{g},\tilde{p}).$$

The physical consequences of this symmetry are by no means obvious. Its investigation has to be left to the future.

Due to the convexity of the set of stochastic matrices we conclude:

Corollary 3 *Let O be an arbitrary object. Let $\hat{O} := (\hat{p},g)$ and $\tilde{O} := (\tilde{p},g)$ two identical systems being in different states. Then $O \geq \hat{O}$ and $O \geq \tilde{O}$ implies*

$$O \geq (\lambda\hat{p} + (1-\lambda)\tilde{p}, g))$$

for every $0 \leq \lambda \leq 1$.

Obviously, it is not satisfactory to restrict the analysis to the quasi-classical case. Fortunately, there are many cases where the investigation of the conversion order can be reduced to the conversion order on the quasi-classical objects and then Theorem 5 is used for proving considerably more general theorems. For that purpose we need a definition and a technical lemma:

Definition 8 *Let $O := (\rho,\gamma)$ be an arbitrary object and B be a basis diagonalizing γ. Let p and g be the vectors given by the diagonal entries of ρ and γ, respectively. Then we define the corresponding quasi-classical object*

$$C_B(O) := (p,g)$$

with respect to the basis B.

Lemma 4 *Let $O := (\rho,\gamma)$ be an arbitrary object. For any basis B diagonalizing γ we have*

$$O \geq C_B(O).$$

Proof: Let B be given by $B := \{|1\rangle, \ldots, |l\rangle\}$. Let σ be the maximally mixed state in l dimensions. Take the equilibrium object $O_e := (\sigma,\sigma)$. With the help of O_e we can obtain $C_B(O)$ by using the resources O: Take the initial state $\rho \otimes \sigma \otimes \gamma$ of the tripartite system $\gamma \otimes \sigma \otimes \gamma$ and perform the transposition

$$|i\rangle \otimes |j\rangle \otimes |k\rangle \;\leftrightarrow\; |k\rangle \otimes |j \oplus i\rangle \otimes |i\rangle,$$

where $\oplus$ denotes the addition modulo l. This transformation is energy conserving since the equilibrium object is degenerated and the other systems have identical level structure. Obviously the transformation transfers the diagonal entries of ρ to the other identical system and destroys the coherence since the coupling to the degenerated ancilla system acts like a measurement. □

We are now able to draw some important conclusions:

Theorem 6 *(partial converse of Theorem 4) If at least one of the two objects $O := (\rho, \gamma)$ and $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ is quasi-classical, i.e.,*

$$[\rho, \gamma] = 0 \quad \text{or} \quad [\tilde{\rho}, \tilde{\gamma}] = 0$$

the following equivalence holds:

$$O \geq \tilde{O}$$

if and only if there is a completely positive trace preserving map fulfilling equations (4) and (5).

Proof: Let $[\rho, \gamma] = 0$. Then we have $[\rho, H] = 0$ for the corresponding Hamiltonian. Take G fulfilling the equations (4) and (5) of Theorem 4. Then we have:

$$0 = G([H, \rho]) = [\tilde{H}, G(\rho)] = [\tilde{H}, \tilde{\rho}].$$

Hence $[\tilde{\rho}, \tilde{\gamma}] = 0$. Hence it is sufficient to show the statement for the case $[\tilde{\rho}, \tilde{\gamma}] = 0$:

Let Q_i and $\tilde{Q}_i$ be the spectral projections of γ and $\tilde{\gamma}$, respectively. Then $P(\sigma) := \sum_i Q_i \rho Q_i$ and $\tilde{P}(\tilde{\sigma}) := \tilde{Q}_i \tilde{\sigma} \tilde{Q}_i$ project any arbitrary density matrix σ and $\tilde{\sigma}$ on its time average with respect to the evolution generated by H and $\tilde{H}$, respectively. Due to the covariance condition of G we conclude

$$G(P(\rho)) = \tilde{P}(G(\rho)) = \tilde{P}(\tilde{\rho}) = \tilde{\rho}.$$

Without loss of generality we can assume that $P(\rho), \gamma, \tilde{\rho}, \tilde{\gamma}$ are diagonal since $[P(\rho), \gamma] = 0$. For any density matrix σ acting on $\mathbb{C}^m$ with arbitrary m let $R(\sigma)$ be the density matrix obtained by cancelling the off-diagonal entries.

We define

$$G' := R \circ G \circ R.$$

Due to $R(P(\rho)) = P(\rho)$ and $R(\tilde{\rho}) = \tilde{\rho}$ we see that G' satisfies the equations (4) and (5) as well. Since G' defines a map from diagonal matrices on diagonal ones it can be described by a stochastic matrix. Therefore we can apply Theorem 5 to show that

$$(R(\rho), \gamma) \geq (\tilde{\rho}, \tilde{\gamma})$$

by taking the canonical basis of $\mathbb{C}^l$ as B. Lemma 4 completes the proof due to the transitivity of the conversion order. □

For $[\tilde{\rho}, \tilde{\gamma}] = 0$ the conversion order can be reduced to the quasi-classical case in the following sense:

Corollary 4 *Let $P(\sigma)$ be (as in the proof of Theorem 6) the time average of any density matrix σ. If $[\tilde{\rho}, \tilde{\gamma}] = 0$ then the following statements are equivalent:*

1. $O := (\rho, \gamma) \geq (\tilde{\rho}, \tilde{\gamma}) =: \tilde{O}$

2. *There is a basis B diagonalizing γ and a basis $\tilde{B}$ diagonalizing $\tilde{\rho}$ and $\tilde{\gamma}$ simultaneously such that*

$$C_B(O) \geq C_{\tilde{B}}(\tilde{O}).$$

3. *For every basis B diagonalizing $P(\rho)$ and γ simultaneously and every basis $\tilde{B}$ diagonalizing ρ and γ simultaneously*

$$C_B(O) \geq C_{\tilde{B}}(\tilde{O})$$

holds.

Proof: $1 \Leftrightarrow 3$: Like in the proof of Theorem 6 there is a stochastic matrix mapping the diagonal entries of $R_B(\rho)$ on the diagonal entries of $R_{\tilde{B}}(\tilde{\rho})$ and the same for the corresponding equilibrium states. $3 \Rightarrow 2$: Obvious. $2 \Rightarrow 1$: The stochastic C matrix mapping the diagonal entries of $R_B(\rho)$ onto the diagonal entries of $\tilde{\rho}$ can be extended to a completely positive trace preserving map by:

$$G := C \circ R_B.$$

Clearly G fulfills the requirements of Theorem 5. □

For generic pairs of objects (ρ, γ) and $(\tilde{\rho}, \tilde{\gamma})$ no difference of the eigenvalues of $\tilde{H}$ will coincide with the eigenvalues of H. One can show that in this case the condition $[\tilde{\rho}, \tilde{\gamma}] = 0$ is necessary:

Lemma 5 *Let the energy levels of the objects $O := (\rho, \gamma)$ and $\tilde{O} := (\tilde{\rho}, \tilde{\gamma})$ be such that no energy difference in O coincides with any difference in $\tilde{O}$. Then $O \geq \tilde{O}$ implies*

$$[\tilde{\rho}, \tilde{\gamma}] = 0.$$

Proof: Let G be the completely positive map required by Theorem 4. Canonically, we extend G to a linear map to the set of matrices acting on the corresponding Hilbert space. Let $|i\rangle$ and $|j\rangle$ be eigenvectors of H with eigenvalues E_i and E_j. Then $|i\rangle\langle j|$ is an eigenvector of the operator $[H, .]$ with eigenvalues $E_i - E_j$. Due to $G([H, .]) = [\tilde{H}, G(.)]$ the density matrix $G(|i\rangle\langle j|)$ has to be an eigenvector of the superoperator $[\tilde{H}, .]$ with eigenvalues $E_i - E_j$ as well. But there are no eigenvectors with this eigenvalue by assumption. Hence $G(|i\rangle\langle j|) = 0$. Hence every density matrix in the image of G commutes with $\tilde{H}$ and $\tilde{\gamma}$. □

Now we will show, that the problem of cooling a qubit is indeed a typical application of the conversion order. In our formal setting we can formulate it as follows: Cooling the qubit down to the temperature $\hat{T}$ means preparing the object

$$\tilde{O} := (\begin{pmatrix} \tilde{p}_1 & 0 \\ 0 & \tilde{p}_2 \end{pmatrix}, \begin{pmatrix} \tilde{g}_1 & 0 \\ 0 & \tilde{g}_2 \end{pmatrix})$$

with

$$\tilde{p}_1 := \frac{1}{1+e^{-E/(k\hat{T})}} \quad \text{and} \quad \tilde{p}_2 = 1 - \tilde{p}_1$$

as well as

$$\tilde{g}_1 = \frac{1}{1+e^{-E/(kT)}} \quad \text{and} \quad \tilde{g}_2 = 1 - \tilde{g}_1.$$

For given resources O it seems hard to decide whether there is a completely positive map as specified by Theorem 6. Fortunately the problem turns out to be equivalent to a well-known problem of testing hypotheses: If one wants to decide whether a given state is the state ρ or the state γ one has to construct a measurement such that the measurement outcome tells whether ρ or γ is more likely. Such a *decision rule* can be described by a *positive operator valued measure* $(\mathcal{E}_\rho, \mathcal{E}_\gamma)$ where $\mathcal{E}_\rho$ and $\mathcal{E}_\gamma$ are positive operators on the resource's Hilbert space with $\mathcal{E}_\rho + \mathcal{E}_\gamma = 1$. Then the risk of the *error of the first kind*, i.e., the risk of deciding ρ if γ is actual, is given by

$$F_1 := tr(\gamma \mathcal{E}_\rho)$$

and the risk of the error of the second kind is given by

$$F_2 := tr(\rho \mathcal{E}_\gamma).$$

If we want to distinguish between the qubit state with temperature T and the state with temperature $\hat{T}$, a straightforward decision rule would be given by measuring whether the system is in its upper or in its lower state. In the first case we will decide to have the higher temperature T, else we decide for $\hat{T}$. This would be a decision rule with the error probabilities

$$F_1 = \frac{e^{-E/(k\hat{T})}}{1+e^{-E/(k\hat{T})}} \quad \text{and} \quad F_2 = \frac{1}{1+e^{-E/(kT)}}. \qquad (10)$$

If the cold qubit has been prepared by using the resources (ρ, γ) one can define a decision rule for the distinction between ρ and γ with the same error probabilities by

$$(\mathcal{E}_{\tilde{\rho}} \circ G, \mathcal{E}_{\tilde{\gamma}} \circ G),$$

where $(\mathcal{E}_{\tilde{\rho}}, \mathcal{E}_{\tilde{\gamma}})$ is the decision rule described above and G is a completely positive trace preserving map with the required properties. Hence the resources (ρ, γ) can only be used for cooling the qubit down to the temperature $\tilde{T}$ if there is a decision rule

$$(\mathcal{E}_\rho, \mathcal{E}_\gamma)$$

with the error probabilities given by equations (10). As one of the main results of our theory, it turns out that this condition is even sufficient:

Theorem 7 *The resource (ρ, γ) can be used for cooling the qubit down to the temperature $\hat{T}$ if and only if there is a decision rule $(\mathcal{E}_\rho, \mathcal{E}_\gamma)$ with $[\mathcal{E}_\gamma, \gamma] = 0$ such that the errors are given by*

$$F_1 = \frac{e^{-E/(k\hat{T})}}{1+e^{-E/(k\hat{T})}}$$

$$F_2 = \frac{1}{1+e^{-E/(kT)}}.$$

Proof: That the condition is necessary has already been explained above.

The other direction can be seen as follows: Define a map from the density matrices on the Hilbert space of O by:

$$G(\sigma) := \begin{pmatrix} tr(\mathcal{E}_\gamma \sigma) & 0 \\ 0 & tr(\mathcal{E}_\rho \sigma) \end{pmatrix}$$

The map G is completely positive since every positive map with a commutative image is completely positive. Furthermore it fulfills the requirements of Theorem 6 (Note that we have $[\mathcal{E}_\gamma, \gamma] = 0$ by assumption). □

One may question the practical importance of the converse direction which states that a cooling procedure is possible if the conditions of Theorem 7 are satisfied, since we used rather sophisticated unitary transformation in the proof of Theorem 6. However, it is not clear whether a more suitable environment (e.g. an infinite dimensional one) might allow optimal transformations which are much more natural. Furthermore it is an important insight that it is not possible to derive any tighter bounds for the resources within our setup.

If any resource object $O := (\rho, \gamma)$ is given and the criterion of Theorem 7 tells that O is not sufficient for obtaining the demanded temperature, it is a natural question whether sufficient cooling is enabled by using many copies of the object O. Therefore one would ask for the least n such that the resource object $O^n := (\rho^{\otimes n}, \gamma^{\otimes n})$ is sufficient for preparing a qubit with temperature $\tilde{T}$. Using Theorem 7, this is the question of the *increase* of the *distinguishability* between the states $\rho^{\otimes n}$ and $\gamma^{\otimes n}$ (see [17]). However, it is important to note that the condition $[\mathcal{E}_\gamma, H] = 0$ in Theorem 6 differentiates the problem from the usual information theoretic questions. — Note that there can be an abundance of basis diagonalizing $\rho^{\otimes n}$ and $\gamma^{\otimes n}$ simultaneously. Therefore the application of Theorem 7 is by no means easy! We will restrict our attention to the quasi-classical case, where we can use essentially Stein's Lemma [18] of classical information theory:

Theorem 8 *For a quasi-classical object $O := (p, g)$ define its Kullback-Leibler Relative Information as*

$$S(g \,\|\, p) := \sum_i g_i \ln \frac{g_i}{p_i}.$$

We consider the situation where the n-fold copy of this resources $O^n := (p^{\otimes n}, g^{\otimes n})$ is used for cooling a two-level system with energy gap E. Let T_n denote the lowest obtainable temperature. Then we have:

$$\lim_{n\to\infty} n\,k\,T_n = E\,S(g \,\|\, p),$$

where k is Boltzmann's constant.

Proof: Let $\tilde{g} := (\tilde{g}_1, \tilde{g}_2)$ be the equilibrium state of the qubit. Let $\mathbf{i} := (i_1, \ldots, i_n) \in \{1, \ldots, l\}^n$ be a pure state in the n-fold copy of the system. Then, instead of working with positive operator valued measurements, we can specify the decision rule by the conditional probabilities

$$w(1|\mathbf{i}) \;\text{ and }\; w(2|\mathbf{i}) = 1 - w(1|\mathbf{i})$$

describing the probability for deciding g or p (respectively) when $\mathbf{i}$ is measured. The corresponding error probabilities are given by

$$F_1 = \sum_{\mathbf{i}} w(2|\mathbf{i})\, g^{\otimes n}(\mathbf{i})$$

and

$$F_2 = \sum_{\mathbf{i}} w(1|\mathbf{i})\, p^{\otimes n}(\mathbf{i}),$$

where we consider the vectors $p^{\otimes n}$ and $g^{\otimes n}$ as probability measures on $\{1, \ldots, l\}^n$ in a straightforward way. Now the proof goes in strong analogy to the proof of Theorem 4.4.4 in [18] with the difference that we have a stochastic decision rule, not a deterministic one. For any $\epsilon > 0$ define the set $B_\epsilon \subset \{1, \ldots, l\}^n$ by

$$B_\epsilon := \{\mathbf{i} |\, S(g \,\|\, p) - \epsilon < \frac{1}{n} \sum_j \ln(g_{i_j}/p_{i_j}) < S(g \,\|\, p) + \epsilon\}$$

Due to the law of large numbers we have:

$$\lim_{n\to\infty} g^{\otimes n}(B_\epsilon) = 1 > \tilde{g}_1$$

Therefore, for large n, we can define a decision rule by

$$w(1|\mathbf{i}) := \frac{\tilde{g}_1}{g^{\otimes n}(B_\epsilon)} \;\; \forall \mathbf{i} \in B_\epsilon$$

and

$$w(1|\mathbf{i}) := 0 \;\; \forall \mathbf{i} \in \{1, \ldots, l\}^n \setminus B_\epsilon.$$

We have

$$\begin{aligned} F_1 &= \sum_{\mathbf{i}} w(2|\mathbf{i})\, g^{\otimes n}(\mathbf{i}) = 1 - \sum_{\mathbf{i}\in B_\epsilon} w(1|\mathbf{i})\, g^{\otimes n}(\mathbf{i}) \\ &= 1 - \tilde{g}_1 = \tilde{g}_2 \end{aligned}$$

as required by Theorem 6. Furthermore we have

$$\begin{aligned} F_2 &= \sum_{\mathbf{i}\in B_\epsilon} w(1|\mathbf{i})\, p^{\otimes n}(\mathbf{i}) \\ &\le \sum_{\mathbf{i}\in B_\epsilon} w(1|\mathbf{i})\, g^{\otimes n}(\mathbf{i}) e^{-n(S(g\,\|\,p)-\epsilon)} = \tilde{g}_1 e^{-n(S(g\,\|\,p)-\epsilon)}. \end{aligned}$$

If the decision rule $w(.|.)$ is defined in any other way, we have

$$\begin{aligned} F_2 &\ge \sum_{\mathbf{i}\in B_\epsilon} w(1|\mathbf{i})\, p^{\otimes n}(\mathbf{i}) \ge \sum_{\mathbf{i}\in B_\epsilon} w(1|\mathbf{i})\, g^{\otimes n}(\mathbf{i})\, e^{-n(S(g\,\|\,p)+\epsilon)} \\ &= \sum_{\mathbf{i}\in B_\epsilon} (1 - w(2|\mathbf{i})) g^{\otimes n}(\mathbf{i})\, e^{-n(S(g\,\|\,p)+\epsilon)} \\ &\ge (g^{\otimes n}(B_\epsilon) - F_1)\, e^{-n(S(g\,\|\,p)+\epsilon)}. \end{aligned}$$

With Theorem 7 we obtain:

$$\begin{aligned} \tilde{g}_1\, e^{-n(S(g\,\|\,p)+\epsilon)} &\ge \frac{e^{-E/(kT_n)}}{1 + e^{-E/(kT_n)}} \\ &\ge (g^{\otimes n}(B_\epsilon) - F_1)\, e^{-n(S(g\,\|\,p)-\epsilon)}. \end{aligned}$$

Since $g^{\otimes n}(B_\epsilon)$ converges to 1 and F_1 is constant we get:

$$\lim_{n\to\infty} n\,k\,T_n = S(g \,\|\, p)\, E.$$

□

V. FURTHER APPLICATIONS OF THE CONVERSION ORDER

One of the big merits of the Second Law of Thermodynamics is the restriction it puts on the efficiency of conversion of heat to other forms of energy: A power station working with two heat reservoirs having temperatures T and $\tilde{T}$ with $\tilde{T} > T$ can never work with an efficiency above

$$\frac{\tilde{T} - T}{\tilde{T}}.$$

We will show in which sense our theory puts restrictions on the efficiency of energy conversion processes which are apparently not given by easy conclusions from the well-known laws of thermodynamics: Assume that we have an energy source, i.e., an object (ρ, γ) such that the mean energy of the state is above the mean energy of equilibrium, i.e., we have

$$tr(H\rho) > tr(H\gamma).$$

Converting the energy to another form of energy means preparing another object $(\tilde{\rho}, \tilde{\gamma})$ by using (ρ, γ) as resource. Generically, we will not expect that it is possible to undo the conversion, i.e., to prepare (ρ, γ) by using now $(\tilde{\rho}, \tilde{\gamma})$ as resource. In general, for a given system $\tilde{\gamma}$, we cannot expect that there is a state $\tilde{\rho}$ such that

$$(\rho, \gamma) \geq (\tilde{\rho}, \tilde{\gamma}) \geq (\rho, \gamma).$$

We can say: The transport of the energy to the other system is an irreversible process so that we cannot regain the original resources. We will illustrate this by an easy example with two qubits:

Take a qubit where the upper level has a higher occupation probability compared to the equilibrium:

$$O := ((p_1, p_2), (g_1, g_2)) \text{ with } p_2 > g_2,$$

where p_2 and g_2 denote the occupation probabilities of the upper level. For another qubit described by the equilibrium probabilities $\tilde{g}_1$ and $\tilde{g}_2$ for the upper and lower level let $\tilde{p}_2$ be the largest probability such that

$$(p, g) \geq (\tilde{p}, \tilde{g}).$$

Assume

$$(p, g) \geq (\tilde{p}, \tilde{g}) \geq (p, g).$$

Then there are stochastic matrices A and B such that

$$BAp = p \text{ and } BAg = g.$$

Since we assume $p \neq g$ the matrix BA must be the identity matrix. Therefore either A and B are identity matrices or A and B are transpositions exchanging the upper and lower state. We can exclude the latter case since that would mean that $\tilde{g}_1 > \tilde{g}_2$ if $g_1 < g_2$ or $\tilde{g}_1 < \tilde{g}_2$ if $g_1 > g_2$. This is not possible for any temperature.

If B and A are identity matrices the energy levels of both systems are compatible. In this case it is obviously possible to transfer the energy without loss. In all the other cases the greatest p_2' such that

$$(p, g) \geq (\tilde{p}, \tilde{g}) \geq ((1 - p_2', p_2'), g)$$

has a value below p_2, i.e., we obtain a lower probability for the upper level compared to the initial one. Of course we can not apply these arguments if many copies of these qubits are available. But even in this case we have the statement that energy conversion with lower loss requires processes involving more qubits at once. Hence energy conversion with high efficiency turns out to be a matter of *complexity* of the conversion process.

VI. COMPARISON WITH LANDAUER'S PRINCIPLE

To elucidate the connection of our analysis with Landauer's principle we reformulate it within our framework.

It should be emphasized that the formulation 'The erasure of one bit of information requires at least the dissipation of the energy $kT \ln 2$.' has to be read in the sense that the bit is in a totally unknown state, i.e., the erasure changes the probabilities of the state $|0\rangle$ from $1/2$ to 1. It is straightforward to model the bit as a two-level system being in its maximally mixed state initially. If we assume the two-level system to be degenerated then the erasure process fits well into our framework since the maximally mixed state is the equilibrium state in this case. Anyway, in the non-degenerate case it would be more complicated to see Landauer's principle since the two-level system may supply the energy required for its own erasure. The requirement of the energy supply $kT \ln 2$ should be made more precisely: Of course this energy cannot be supplied by the *heat* of an reservoir having the temperature T, since heat is a useless form of energy. We rather need *free energy* for driving the process. Therefore, we need resources (p, g) such that the free energy of p exceeds the free energy of g at by least $kT \ln 2$. Note that this difference of the free energies of p and g is given by the Kullback-Leibler Information up to Boltzmann's constant:

The free energy of any state p with respect to the inverse temperature β is given by:

$$F_g(p) := E_g(p) - \frac{1}{\beta} S(p),$$

where $S(p) := -\sum_i p_i \ln p_i$ is the entropy and $E_g(p)$ is the mean energy in the state p (in view of the energy level structure defined by g), i.e.

$$E_g(p) := \sum_i p_i E_i.$$

Easy calculation shows the following well-known result:

$$F_g(p) - F_g(g) = \frac{1}{\beta}(\sum_i p_i \ln(p_i/g_i)) = \frac{1}{\beta} S(p \,\|\, g).$$

Note that here (in contrast to Theorem 8) the relative information $S(p \,\|\, g)$ instead of $S(g \,\|\, p)$ occurs! Therefore, we rephrase Landauer's principle as: 'The erasure process (in the sense above) requires an object (p, g) with $S(p \,\|\, g) \geq \ln 2$'. In order to show this, we will need the following Lemma:

Lemma 6 *For arbitrary objects* (p, g) *and* $(\tilde{p}, \tilde{g})$

$$(p, g) \geq (\tilde{p}, \tilde{g})$$

implies

$$S(p \,\|\, g) \geq S(\tilde{p} \,\|\, \tilde{g})$$

and

$$S(g \,\|\, p) \geq S(\tilde{g} \,\|\, \tilde{p}).$$

Proof: It is well-known that $S(.\|.)$ is a distance measure on the set of probability measures which is decreasing with respect to stochastic maps (Uhlmann's monotonicity theorem [19]). □

Corollary 5 *('Landauer's principle') To obtain the perfectly initialized bit $\tilde{p} = (0,1)$ from the maximally unknown bit $\tilde{g} = (1/2, 1/2)$ one needs resources (p, g) with $S(p \,\|\, g) \geq \ln 2$, i.e,*

$$(p, g) \geq (\tilde{p}, \tilde{g})$$

implies

$$S(p \,\|\, g) \geq \ln 2.$$

This can be seen by checking the equality $S(\tilde{p} \,\|\, \tilde{g}) = \ln 2$.

Corollary 6 *('Perfect erasure is impossible with generic resources') Let p be a state with $p_i \neq 0$ for every i. Then there is no n such that*

$$(p^{\otimes n}, g^{\otimes n}) \geq (\tilde{p}, \tilde{g}),$$

with $\tilde{p} = (0,1)$ and $\tilde{g} = (1/2, 1/2))$. This can be seen by $S(\tilde{g} \,\|\, \tilde{p}) = \infty \neq S(g^{\otimes n} \,\|\, p^{\otimes n})$.

Note that Landauer's principle is arguing with the relative entropy $S(p \,\|\, g)$ whereas our analysis uses $S(g \,\|\, p)$. This exchange of the role of p and g is more important than it seems: Both quantities measure the distance from the equilibrium state, but with respect to the first distance measure the states $p := (\epsilon, 1-\epsilon)$ and $p' := (1,0)$ have almost the same distance from equilibrium if ϵ is small. In contrast, the distance measure obtained by exchanging the role between p and g, converges to infinity as ϵ tends to 0.

Therefore, $S(g \,\|\, p)$ seems more appropriate for describing the difficulties in approaching the absolute Zero! In other words: The usual thermodynamic quantities like energy, free energy and entropy cannot explain 'the hardness of the struggle against the last milli-Kelvin above the absolute Zero'.

VII. WHAT IS THE KULLBACK-LEIBLER INFORMATION OF A TYPICAL ENERGY SOURCE?

One may rephrase our results by the statement 'for reliable bit erasure one needs much more than the free energy $\ln 2kT$'. But this formulation is misleading: Even for arbitrarily reliable bit erasure, there cannot exist any lower bound tighter than the one given by Landauer: If the resource's state is a pure one it may enable perfect erasure even with the free energy $\ln 2kT$. This statement is trivial since any qubit can be prepared into a perfect pure state if the resource is given by a qubit with the identical energy gap as the first one being in a pure state. This example seems to be unserious since it shifts the problem of cooling to the problem of supplying resources with the same temperature. Furthermore the problem of cooling seems to have a circular logical structure. Nevertheless the example shows, that any statements about tighter bounds have to refer to particular assumptions about the statistical properties of the energy source's state.

In view of this, we rephrase our results more carefully: Given any resource object $O := (\rho, \gamma)$ with the property that no eigenvalue of ρ is 0. Then an arbitrarily reliable bit erasure process requires arbitrary many copies of O, i.e., we need the resources O^n with appropriately large n, even if the free energy of O^m exceeds $\ln kT$ already for a considerably smaller number m. For making definite statements about n and m one should make assumptions about ρ and γ and fix the demanded error probability. Deriving statistical properties of the states of realistic energy sources is not easy and should be a subject of further research. However, from a quite fundamental point of view, it is quite natural to ask for the 'thermodynamic worth' of a *heat source* with respect to good cooling and reliable bit erasure: We assume that the resource's state ρ is a thermal equilibrium state with temperature $\tilde{T} > T$. This assumption is an example of a non-circular way of treating the problem of the required resources: The resource's state is prepared by controlling *macroscopic* quantities (in our example the temperature) without any direct possibility of controlling its *microphysical* state. We show that in our example the relative information can be calculated explicitly if the partition function of the energy source is known:

Lemma 7 *Let (p, g) be an object where p is an equilibrium state for the inverse temperature $\tilde{\beta}$ and g is the equilibrium state for the environment's inverse temperature β. With the partition function*

$$Z(\beta) := \sum_i e^{-\beta E_i}$$

we have:

$$p_i = e^{-\tilde{\beta} E_i}/Z(\tilde{\beta}), \;\; g_i = e^{-\beta}/Z(\beta).$$

Hence we get the Kullback-Leibler Information

$$\begin{aligned} S(g \,\|\, p) &= \sum g_i \ln(g_i/p_i) \\ &= \ln Z(\tilde{\beta}) - \ln Z(\beta) + E_g(g)(\tilde{\beta} - \beta), \end{aligned}$$

where $E_g(g)$ is the mean energy of the equilibrium state g. This term is clearly finite for β and $\tilde{\beta}$ being finite. Hence the required number of copies of the heat source (p, g) for cooling down to the demanded temperature can be estimated by knowing the temperatures and the partition function.

VIII. CONCLUSIONS

To investigate the problem of cooling from a quite fundamental point of view our model includes the driving energy source as a quantum system with density matrix describing its statistical state. This setup elucidated the lacks of the traditional thermodynamic laws for explaining the resource requirements for cooling processes approaching the ground states: It is by no means sufficient that the energy source is able to supply enough free energy, it rather is necessary, that the density matrix of the energy source has a large enough distance from its equilibrium state in another information theoretic sense. One has to distinguish between two different questions: Firstly one wants to determine whether a qubit can be cooled down even further if it is already colder than the environment's temperature. This problem turned out to be essentially a geometric one and we have shown, that the limit temperature at which every cooling process breaks down is given by a simple parameter which we called 'maximal diagonal deviation' from equilibrium. If one starts with a qubit having environment temperature, this limit temperature can in general only be approached by repeating a cooling procedure with refreshed resources at each cycle.

The second problem is to determine the temperature which can be obtained by starting with a qubit with the environment's temperature if no such refreshment of the resources is allowed. Here the determination of the possibilities of cooling is essentially equivalent to the determination of an optimal decision rule which can distinguish between the resources density matrix and the corresponding equilibrium density matrix. This result strongly emphasizes the fact that information theoretical arguments can rule out physical processes in a way which goes far beyond usual entropy arguments.

In a straightforward way, our theory applies to the more general question of the resources needed for preparing approximately pure states in any multi-level quantum system. This justifies the quite general formulation of the title: The thermodynamic costs of *reliability*.

IX. APPENDIX

For the proof of Lemma 1 we need the following technical lemma:

Lemma 8 *Let $A := diag(a_1, \ldots, a_n)$ with $a_1 \geq a_2 \geq \ldots \geq a_n$ and $B := diag(b_1, \ldots, b_n)$ with $b_i = -1$ for $i \leq l$ and $b_i = 1$ for $i > l$.*

Let u be an arbitrary unitary operator. Then

$$tr(AuBu^*) \geq tr(AB).$$

Proof: We have:

$$\begin{aligned} & tr(AuBu^*) - tr(AB) \\ &= \sum_j a_j \sum_i b_i(|u_{ji}|^2 - \delta_{ij}) \\ &= \sum_j a_j (\sum_{i \neq j} b_i |u_{ji}|^2 - b_j \sum_{i \neq j} |u_{ji}|^2), \end{aligned} \tag{11}$$

where we have used $\sum_j |u_{ji}|^2 = 1$ since u is unitary. The term in equation (11) reads as:

$$\sum_j a_j \sum_{i \neq j} |u_{ji}|^2 (b_i - b_j) = \tag{12}$$

$$\sum_{j=1}^{l} a_j \sum_{i=l+1}^{n} |u_{ji}|^2 2 + \sum_{j=l+1}^{n} a_j \sum_{i=1}^{l} |u_{ji}|^2 (-2) \geq \tag{13}$$

$$2a_l \sum_{j=1}^{l} \sum_{i=l+1}^{n} |u_{ji}|^2 - 2a_{l+1} \sum_{j=l+1}^{n} \sum_{i=1}^{l} |u_{ji}|^2. \tag{14}$$

This term is greater or equal than zero since the double sums are the same: Because u is a unitary operator, the row square sums as well as the column sums equal 1. Therefore,

$$\sum_{j+1}^{l} \sum_{i=l+1}^{n} |u_{ji}|^2 = l - \sum_{i,j \leq l} |u_{ji}|^2 = \sum_{j=l+1}^{n} \sum_{i=1}^{l} |u_{ji}|^2.$$

□

Now we are able to prove Lemma 1:

Proof: u commutes with $\gamma \otimes \sigma$ and hence with its spectral projections. Therefore we have

$$u = \sum u_j \quad \text{with} \quad u_j := \sum P_j u P_j.$$

Then it is sufficient to show

$$tr(u_j \alpha u_j^* (1 \otimes \sigma_z)) \leq tr(P_j \alpha P_j (1 \otimes \sigma_z)).$$

Since

$$tr(u_j \alpha^* u_j (1 \otimes \sigma_z)) = tr(u_j \alpha u_j^* P_j (1 \otimes \sigma_z) P_j),$$

we can reduce the problem completely to the situation of Lemma 8 by considering the range of every P_j separately: Restricted to the range of P_j, the operator u_j acts as a unitary one. □

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